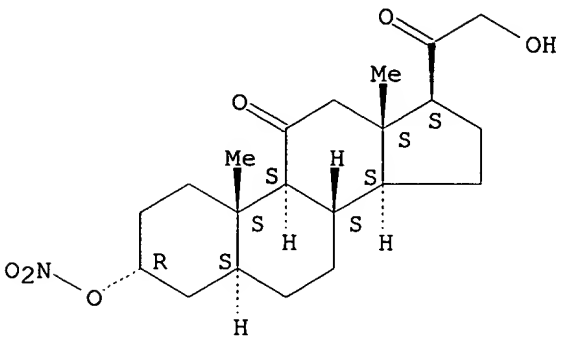
L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-hydroxy-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
MF **C21 H31 N O6**

Absolute stereochemistry.

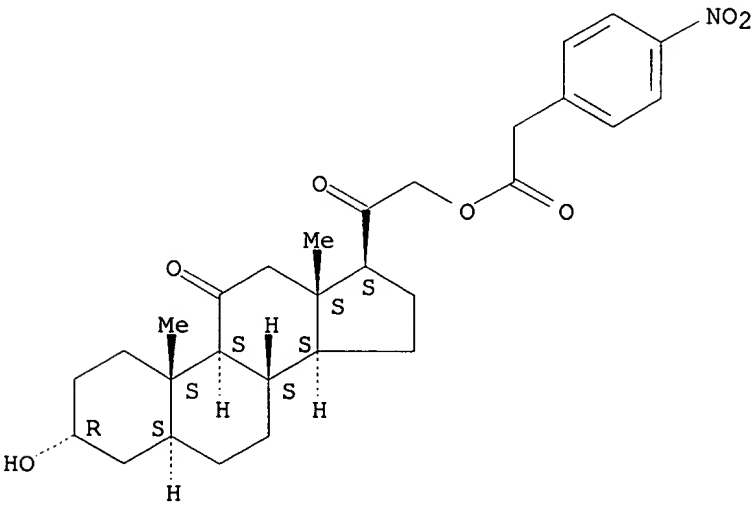


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):17

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 3-hydroxy-21-[[(4-nitrophenyl)acetyl]oxy]-,
(3.alpha.,5.alpha.)- (9CI)
MF **C29 H37 N O7**

Absolute stereochemistry.

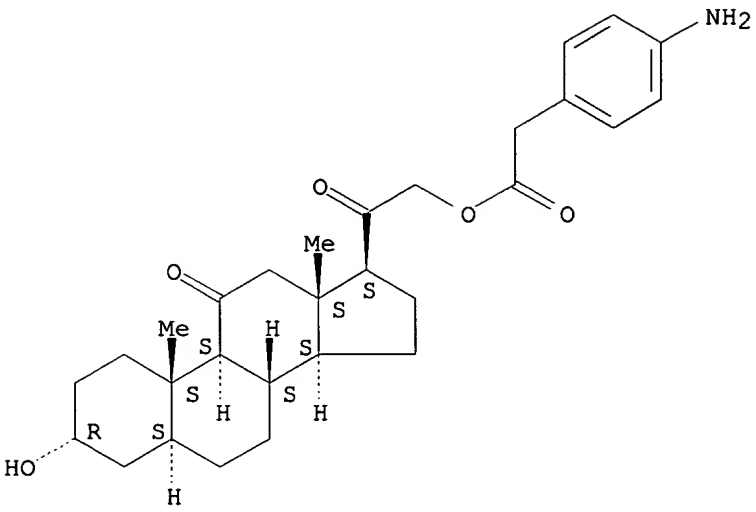


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-[[(4-aminophenyl)acetyl]oxy]-3-hydroxy-,

(3.alpha.,5.alpha.)- (9CI)
MF **C29 H39 N O5**

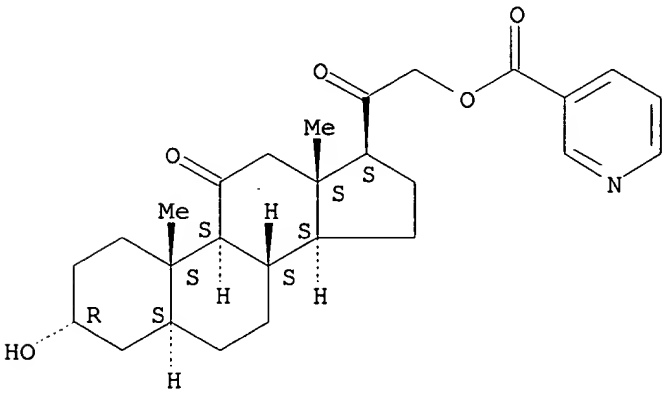
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 3-hydroxy-21-[(3-pyridinylcarbonyl)oxy]-, (3.alpha.,5.alpha.)- (9CI)
MF **C27 H35 N O5**

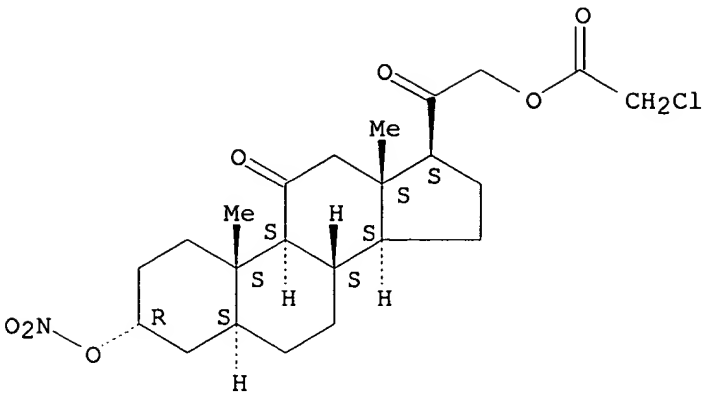
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-[(chloroacetyl)oxy]-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
MF **C23 H32 Cl N O7**

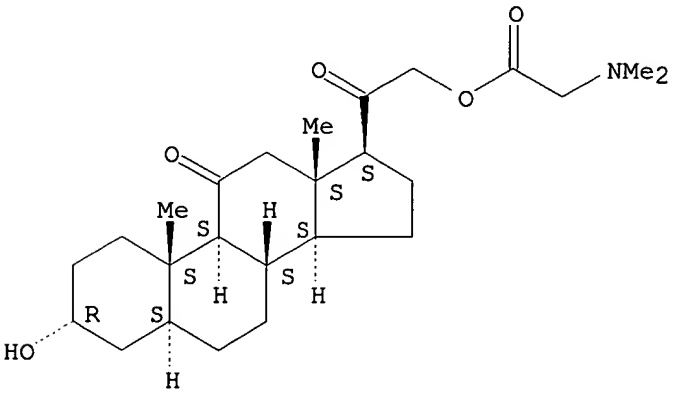
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, N,N-dimethyl-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester (9CI)
MF **C25 H39 N O5**

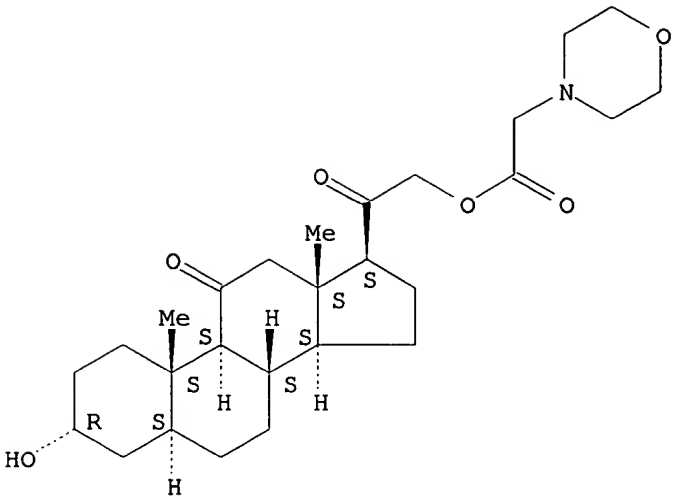
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 3-hydroxy-21-[(4-morpholinylacetyl)oxy]-, (3.alpha.,5.alpha.)- (9CI)
MF **C27 H41 N O6**

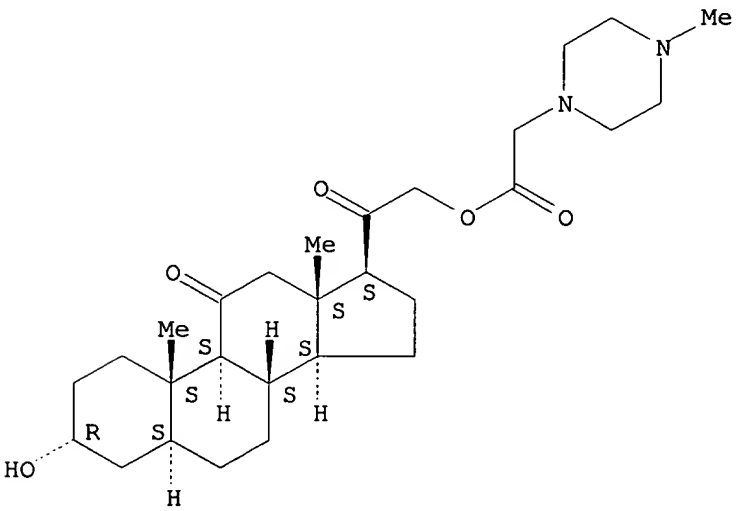
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 3-hydroxy-21-[[(4-methyl-1-piperazinyl)acetyl]oxy]-, (3.alpha.,5.alpha.)- (9CI)
MF **C28 H44 N2 O5**

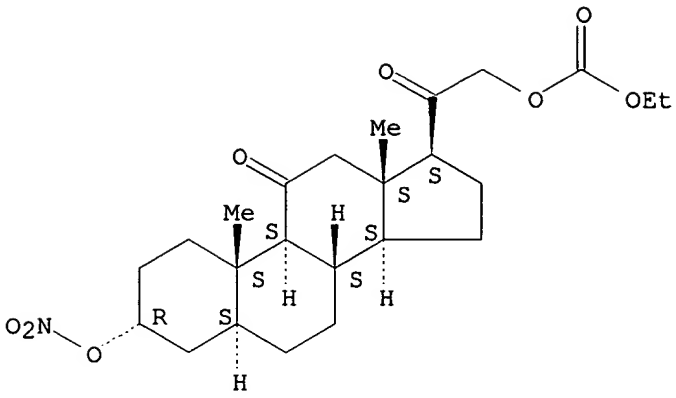
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-[(ethoxycarbonyl)oxy]-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
MF **C24 H35 N O8**

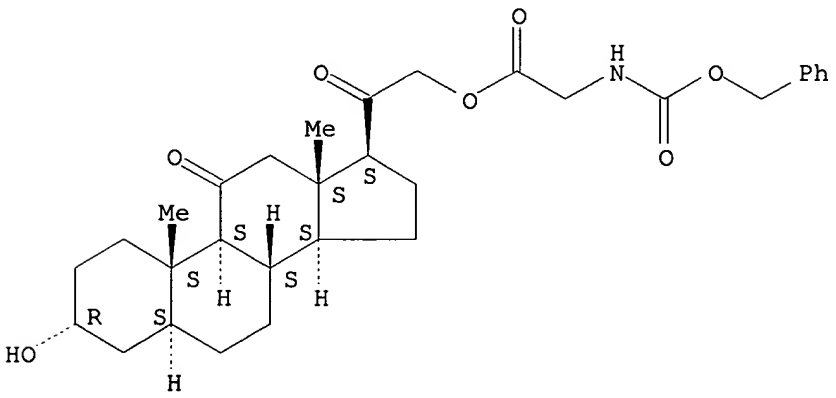
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, N-[(phenylmethoxy)carbonyl]-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester (9CI)
MF **C31 H41 N O7**

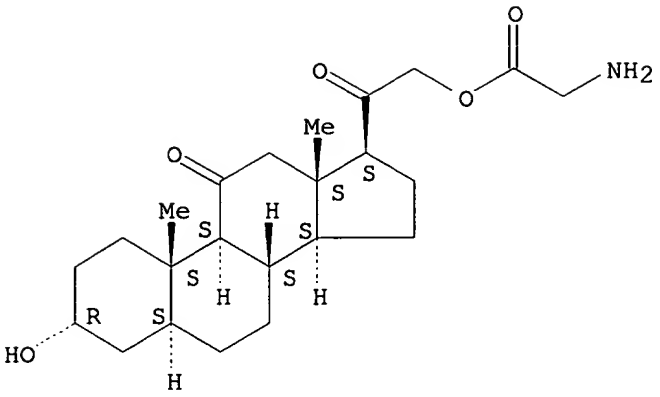
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester, hydrochloride (9CI)
MF **C23 H35 N O5 . Cl H**

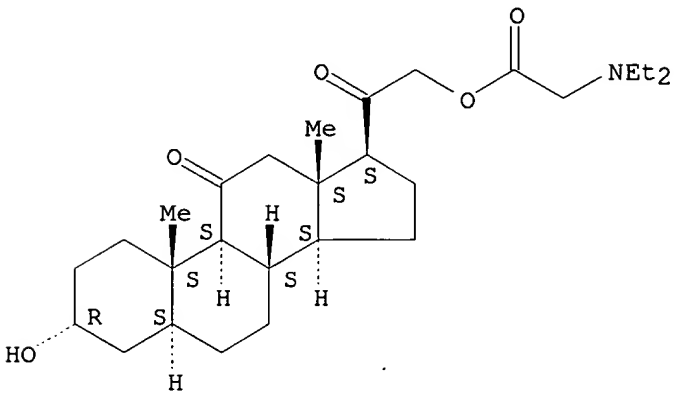
Absolute stereochemistry.



● HCl

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, N,N-diethyl-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester (9CI)
MF **C27 H43 N O5**

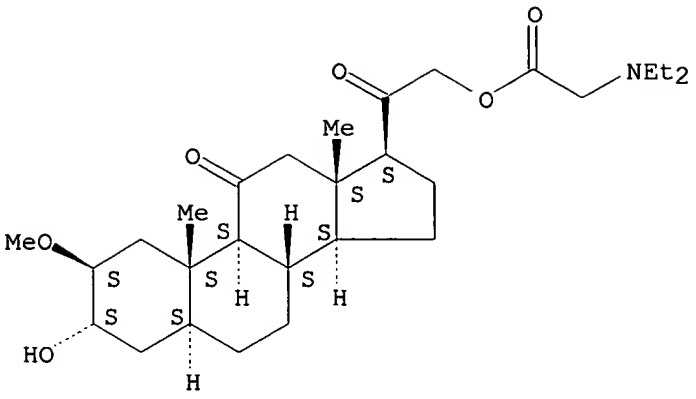
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, N,N-diethyl-, (2.beta.,3.alpha.,5.alpha.)-3-hydroxy-2-methoxy-11,20-dioxopregnan-21-yl ester (9CI)
MF **C28 H45 N O6**

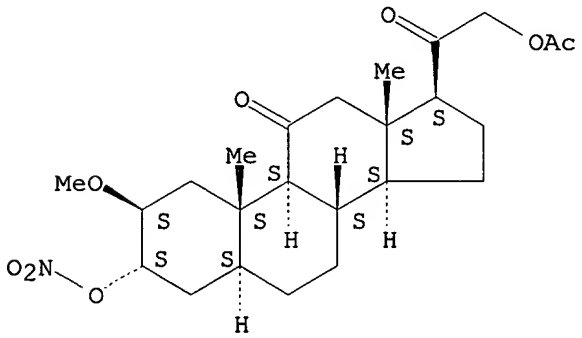
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-(acetyloxy)-2-methoxy-3-(nitrooxy)-, (2.beta.,3.alpha.,5.alpha.)- (9CI)
MF **C24 H35 N O8**

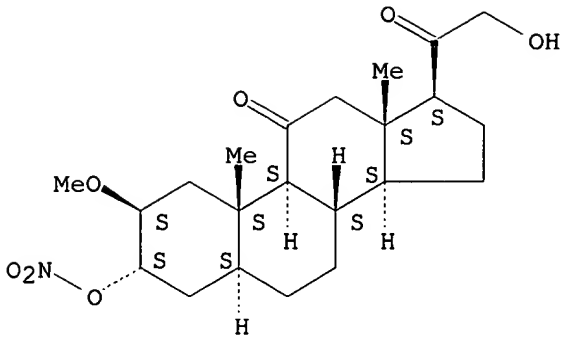
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-hydroxy-2-methoxy-3-(nitrooxy)-, (2.beta.,3.alpha.,5.alpha.)- (9CI)
MF **C22 H33 N O7**

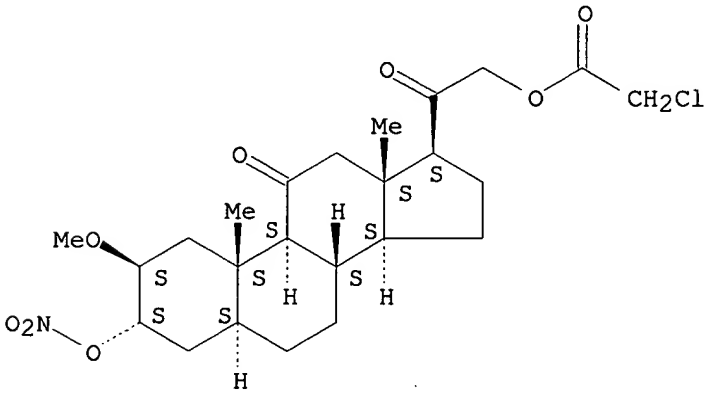
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-[(chloroacetyl)oxy]-2-methoxy-3-(nitrooxy)-, (2.beta.,3.alpha.,5.alpha.)- (9CI)
MF **C24 H34 Cl N O8**

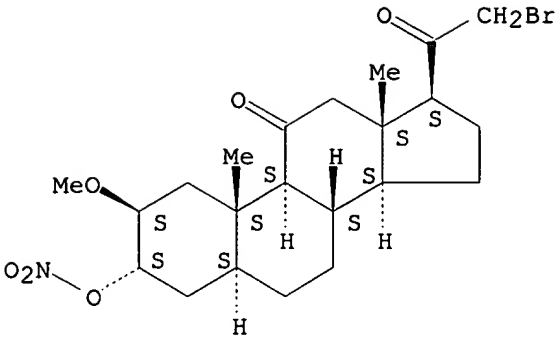
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-bromo-2-methoxy-3-(nitrooxy)-, (2.beta.,3.alpha.,5.alpha.)- (9CI)
MF **C22 H32 Br N O6**

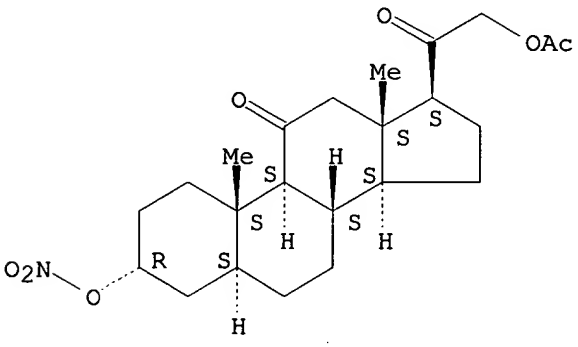
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-(acetyloxy)-3-(nitrooxy)-, (3.alpha.,5.alpha.)-(9CI)
MF **C23 H33 N O7**

Absolute stereochemistry.

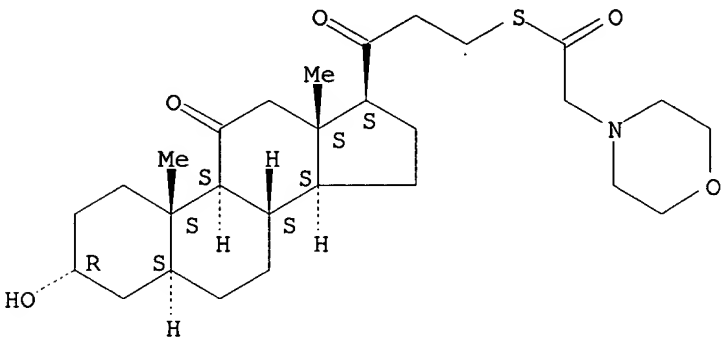


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-[(4-morpholinylacetyl)thio]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C28 H43 N O5 S**

Absolute stereochemistry.



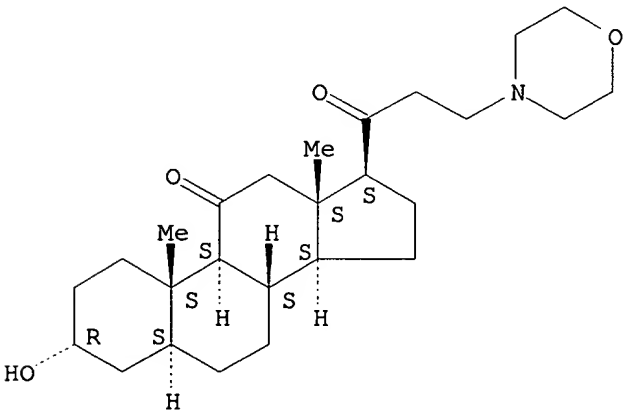
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):28

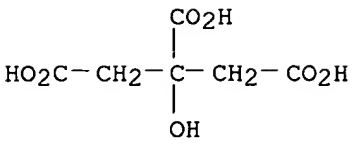
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1) (9CI)
MF **C26 H41 N O4 . 1/3 C6 H8 O7**

CM 1

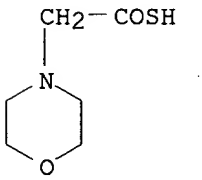
Absolute stereochemistry.



CM 2



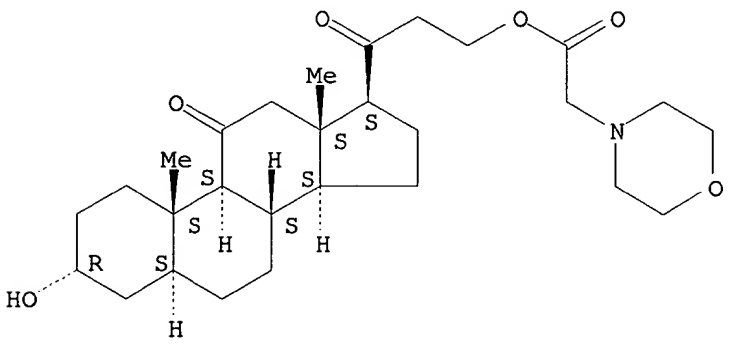
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 4-Morpholineethanethioic acid (9CI)
MF **C6 H11 N O2 S**



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

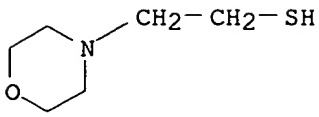
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-[(4-morpholinylacetyl)oxy]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C28 H43 N O6**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

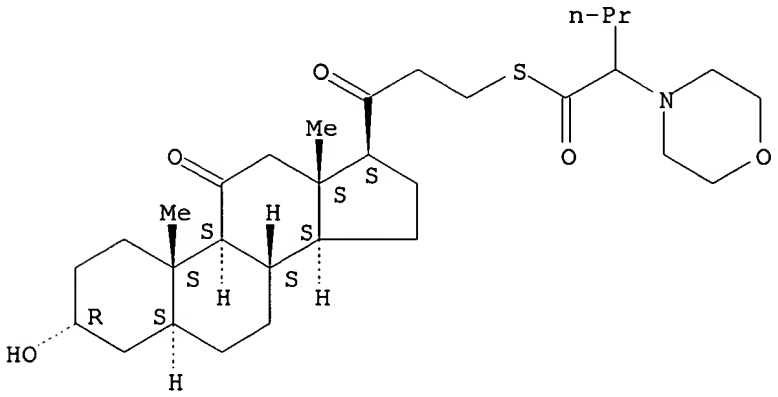
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 4-Morpholineethanethiol (6CI, 7CI, 8CI, 9CI)
MF **C6 H13 N O S**
CI COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

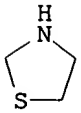
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-[[2-(4-morpholinyl)-1-oxopentyl]thio]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C31 H49 N O5 S**

Absolute stereochemistry.



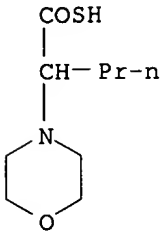
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Thiazolidine (6CI, 7CI, 8CI, 9CI)
MF **C3 H7 N S**
CI COM, RPS



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

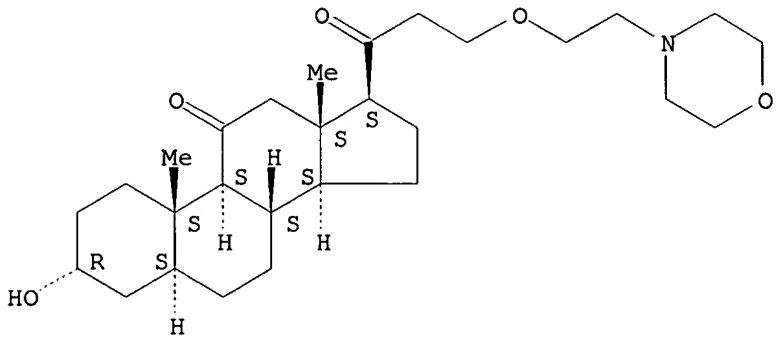
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 4-Morpholineethanethioic acid, .alpha.-propyl- (9CI)
MF **C9 H17 N O2 S**



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-[2-(4-morpholinyl)ethoxy]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C28 H45 N O5**

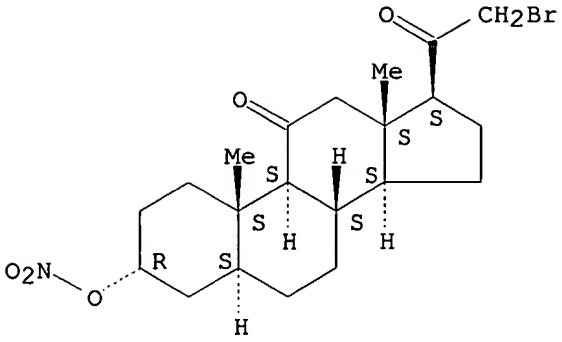
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnane-11,20-dione, 21-bromo-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
MF **C21 H30 Br N O5**

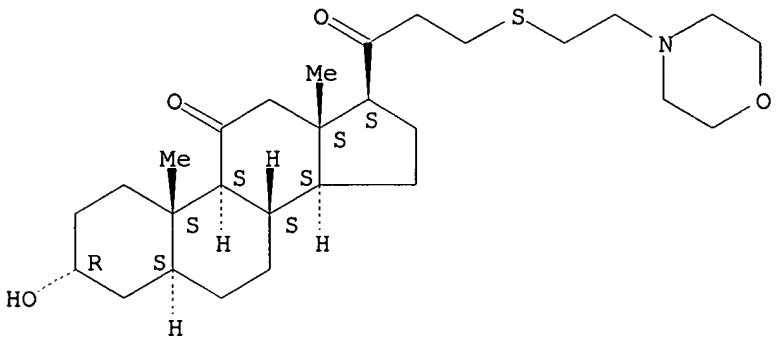
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

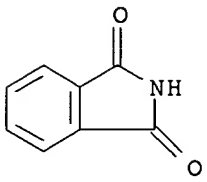
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-[[2-(4-morpholinyl)ethyl]thio]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C28 H45 N O4 S**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

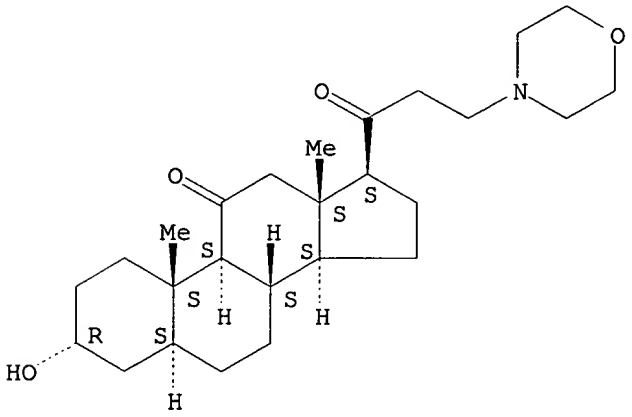
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1H-Isoindole-1,3(2H)-dione, potassium salt (9CI)
MF **C8 H5 N O2 . K**
CI COM



● K

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C26 H41 N O4**
CI COM

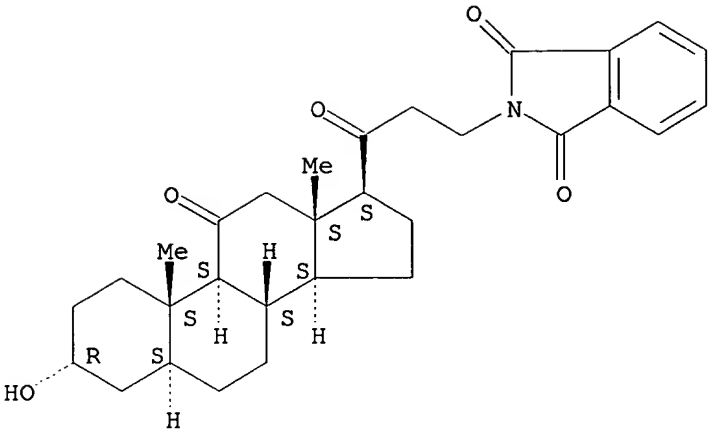
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

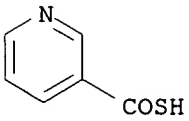
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1H-Isoindole-1,3(2H)-dione, 2-[3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-oxopropyl]- (9CI)
MF **C30 H37 N O5**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

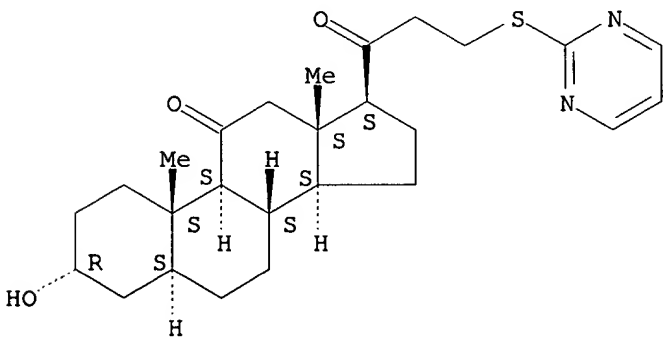
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 3-Pyridinecarbothioic acid (9CI)
MF **C6 H5 N O S**
CI COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

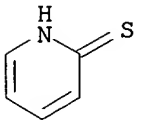
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(2-pyrimidinylthio)propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C26 H36 N2 O3 S**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

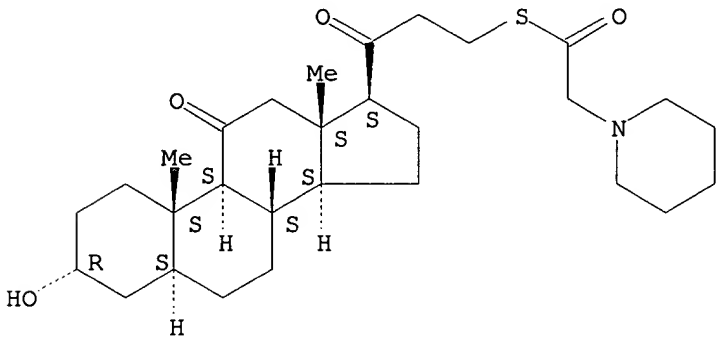
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 2(1H)-Pyridinethione (6CI, 7CI, 8CI, 9CI)
MF **C5 H5 N S**
CI COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-[(1-piperidinylacetyl)thio]propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C29 H45 N O4 S**

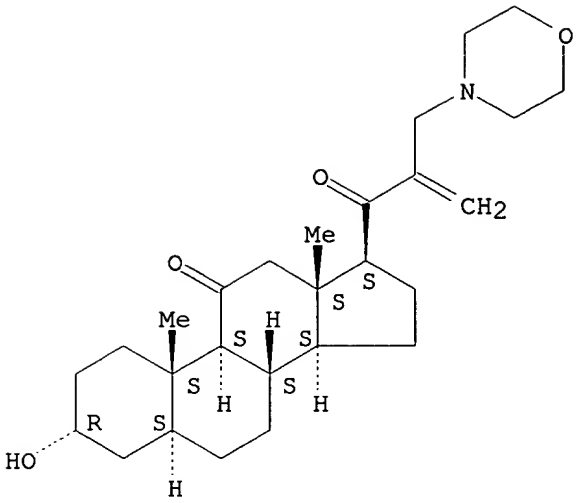
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

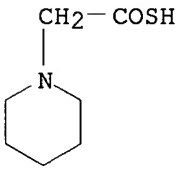
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[2-(4-morpholinylmethyl)-1-oxo-2-propenyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C27 H41 N O4**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

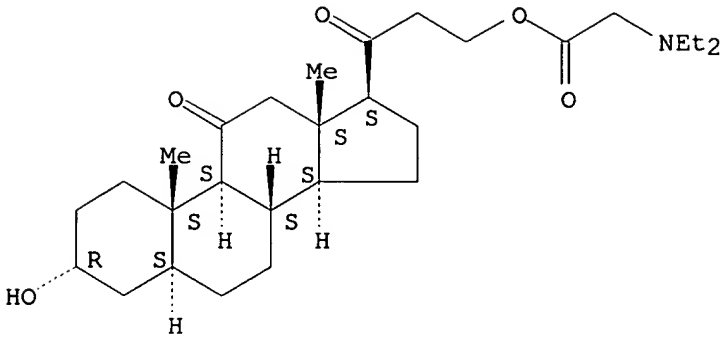
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Piperidineethanethioic acid (9CI)
MF **C7 H13 N O S**



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Glycine, N,N-diethyl-, 3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-oxopropyl ester (9CI)
MF **C28 H45 N O5**

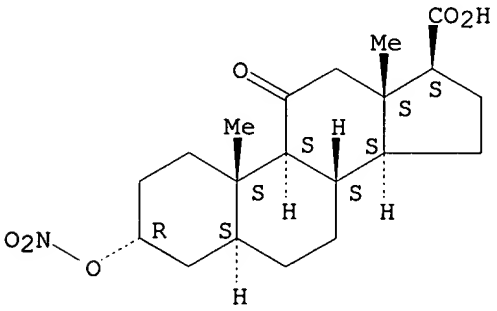
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstane-17-carboxylic acid, 3-(nitrooxy)-11-oxo-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C20 H29 N O6**

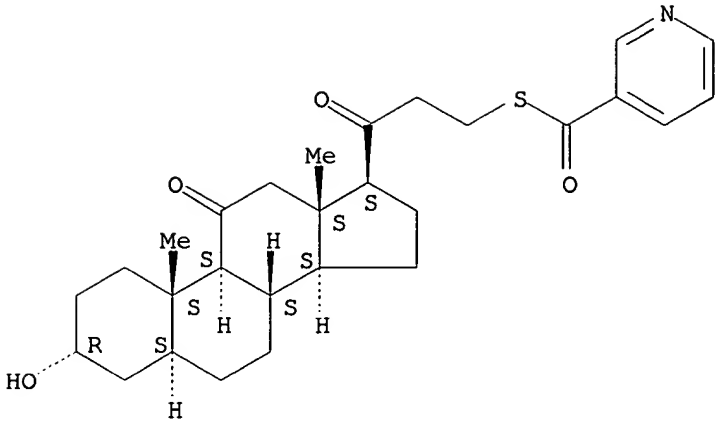
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

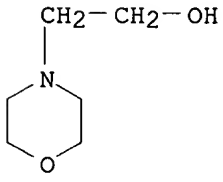
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-[(3-pyridinylcarbonyl)thio]propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C28 H37 N O4 S**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

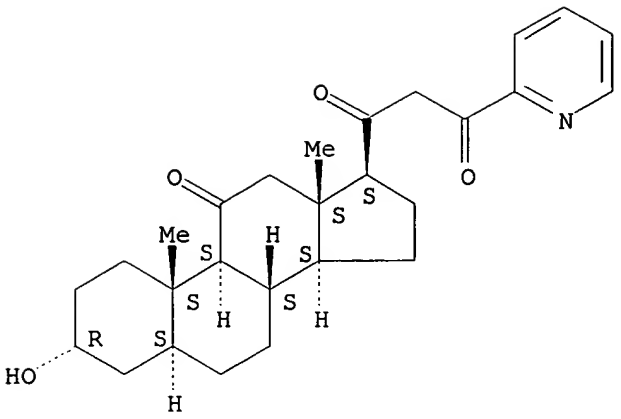
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 4-Morpholineethanol (6CI, 7CI, 8CI, 9CI)
MF **C6 H13 N O2**
CI COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1,3-Propanedione, 1-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-(2-pyridinyl)- (9CI)
MF **C27 H35 N O4**

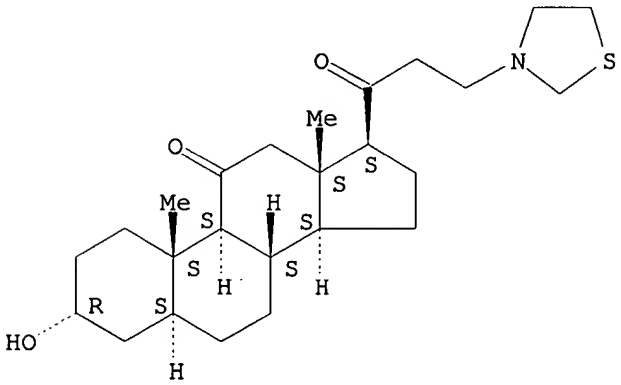
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(3-thiazolidinyl)propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C25 H39 N O3 S**

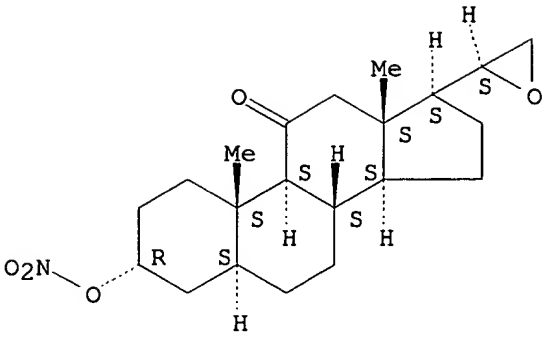
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pregnan-11-one, 20,21-epoxy-3-(nitrooxy)-, (3.alpha.,5.alpha.,20S)- (9CI)
MF **C21 H31 N O5**

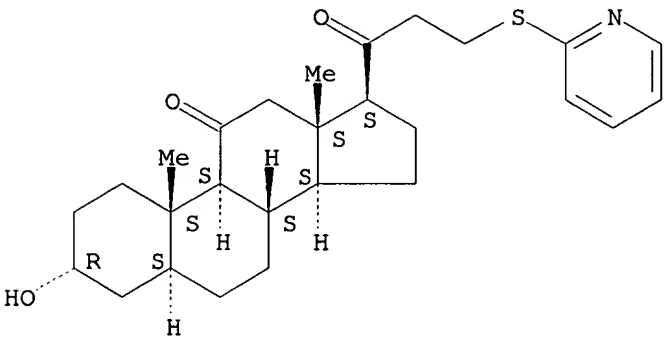
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

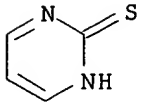
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(2-pyridinylthio)propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
MF **C27 H37 N O3 S**

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 2(1H)-Pyrimidinethione (8CI, 9CI)
MF **C4 H4 N2 S**
CI COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> d ibib ab hitstr 1-2

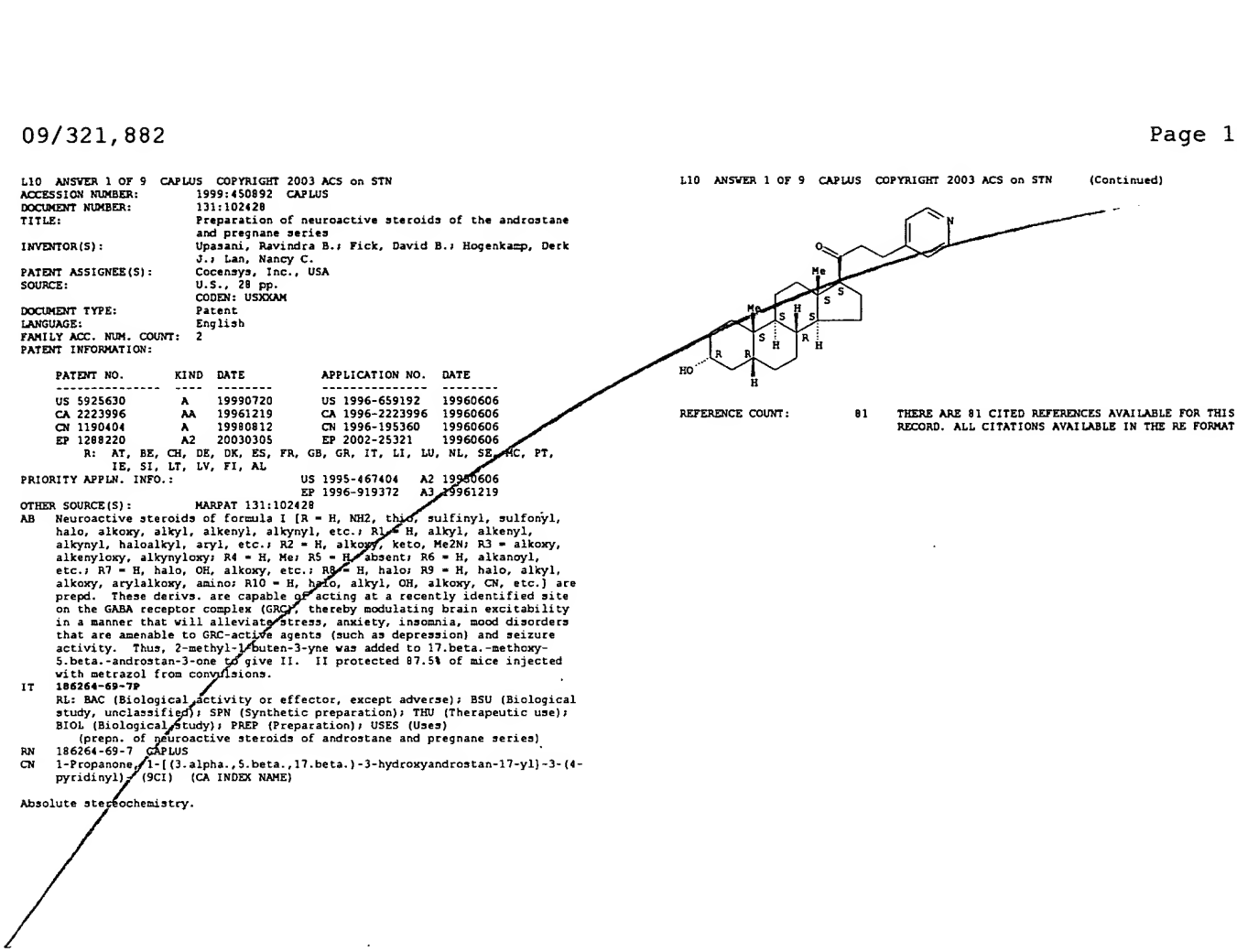
L10 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:450892 CAPLUS
DOCUMENT NUMBER: 131:102428
TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: U.S., 28 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5925630 | A | 19990720 | US 1996-659192 | 19960606 |
| CA 2223996 | AA | 19961219 | CA 1996-2223996 | 19960606 |
| CN 1190404 | A | 19980812 | CN 1996-195360 | 19960606 |
| EP 1208220 | A2 | 20030305 | EP 2002-25321 | 19960606 |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL

PRIORITY APPLN. INFO.: US 1995-467404 A2 19950606
EP 1996-919372 A3 19961219
OTHER SOURCE(S): MARPAT 131:102428
AB Neuroactive steroids of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halo, alkoxy, alkyl, alkenyl, alkynyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, aryl, etc.; R2 = H, alkoxy, keto, Me2N; R3 = alkoxy, alkenyloxy, alkynyloxy; R4 = H, Me; R5 = H, absent; R6 = H, alkanoyl, etc.; R7 = H, halo, OH, alkoxy, etc.; R8 = H, halo; R9 = H, halo, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halo, alkyl, OH, alkoxy, CN, etc.] are prepd. These derivs. are capable of acting at a recently identified site on the GABA receptor complex (GRC), thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.beta.-methoxy-5.beta.-androstan-3-one to give II. II protected 87.5% of mice injected with metrazol from convulsions.
IT **186264-69-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neuroactive steroids of androstane and pregnane series)
RN 186264-69-7 CAPLUS
CN 1-Propanone, 1-[(3.alpha.,5.beta.,17.beta.)-3-hydroxyandrostan-17-yl]-3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:112239 CAPLUS
DOCUMENT NUMBER: 128:188632
TITLE: Use of GABA agonists and NMDA receptor antagonists for the treatment of migraine headache
INVENTOR(S): Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA; Lan, Nancy C.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

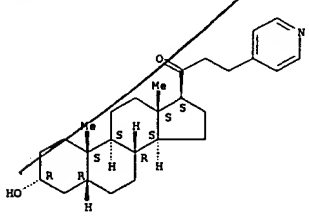
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9805337 | A1 | 19980212 | WO 1997-US13430 | 19970731 |

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| AU 9739672 | A1 | 19980225 | AU 1997-39672 | 19970731 |

PRIORITY APPLN. INFO.: US 1996-22937P P 19960801
WO 1997-US13430 W 19970731
AB Methods are disclosed for treating or preventing migraine headache by administering to an animal a GABA receptor agonist (e.g. a neuroactive steroid) and/or an NMDA receptor antagonist (e.g. a dihydroquinoxaline deriv.). Also disclosed are pharmaceutical compns. and kits for the treatment or prevention of migraine headache.
IT **186264-69-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(GABA agonists and NMDA receptor antagonists for migraine headache treatment)
RN 186264-69-7 CAPLUS
CN 1-Propanone, 1-[(3.alpha.,5.beta.,17.beta.)-3-hydroxyandrostan-17-yl]-3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

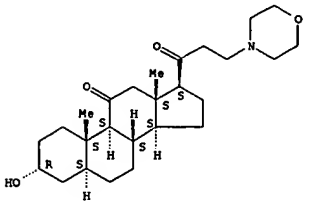
Absolute stereochemistry.



L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

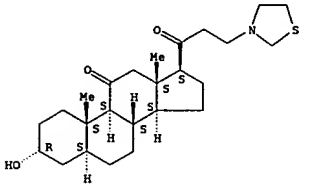
L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51228-28-5 CAPLUS
CN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(3-thiazolidinyl)propyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

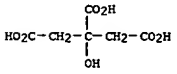
Absolute stereochemistry.



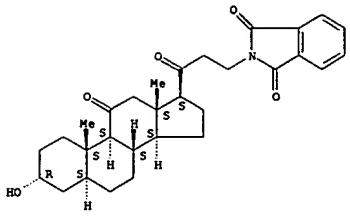
RN 51228-32-1 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

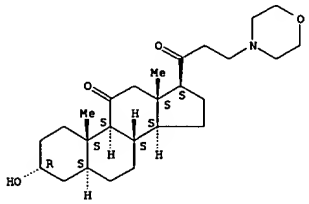


RN 51228-33-2 CAPLUS
CN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1) (9CI) (CA INDEX NAME)

CM 1

CRN 51228-01-4
CMF C26 H41 N O4

Absolute stereochemistry.



CM 2

CRN 77-92-9
CMF C6 H8 O7

L10 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1972:514701 CAPLUS
DOCUMENT NUMBER: 77:114701
TITLE: 3.alpha.-Hydroxy-5.alpha.-pregnane-11,20-diones
INVENTOR(S): Phillipps, Gordon Hanley; Newall, Christopher Earle
PATENT ASSIGNEE(S): Glaxo Laboratories Ltd.
SOURCE: Ger. Offen., 45 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2162594 | A | 19720706 | DE 1971-2162594 | 19711216 |
| NL 7117249 | A | 19720620 | NL 1971-17249 | 19711216 |
| FR 2118118 | A5 | 19720728 | FR 1971-45226 | 19711216 |
| FR 2118118 | B1 | 19751128 | | |
| US 3882151 | A | 19750506 | US 1971-208961 | 19711216 |
| CA 995662 | A1 | 19760824 | CA 1971-130271 | 19711216 |
| US 3969345 | A | 19760713 | US 1975-551315 | 19750220 |

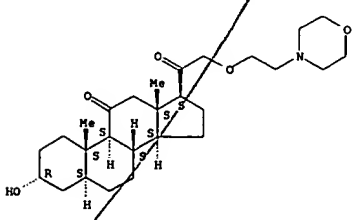
PRIORITY APPLN. INFO.: GB 1970-60065 19701217
US 1971-208961 19711216

AB Twenty title compds. [I, R = H2, O; R1 = H, Ac, O2N; R2 = H, Me; R3 = H, .beta.-MeO, .alpha.-OH, R4 = OMe, OEt, OCHMe2, O(CH2)2OMe, OC6H4NH2-p, O(CH2)2Cl, 2-morpholinoethoxy, 2-(4-methylpiperazinyl)ethoxy, O(CH2)2CN, O(CH2)2CO2Et, O(CH2)2Cl, O(CH2)3Cl, OCH2Ph, cyclohexyloxy], useful was anesthetics, were prepd. by methylation of the corresponding 21-diazo compd. Thus, 21-diazo-3.beta.-nitrato-5.alpha.-pregnane-11,20-dione in dry CH2Cl2-MeOH was refluxed with 14% BF3.MeOH 25 min to give I (R = O, R1 = NO2, R2 = R3 = H, R4 = OMe), which was stirred with Zn powder in HOAc 1.5 hr to give I (R = O, R1 = R2 = R3 = H, R4 = OMe).

IT 38601-40-0P 38601-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

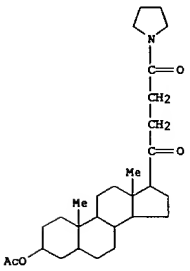
RN 38601-40-0 CAPLUS
CN Pregnane-11,20-dione, 3-hydroxy-21-[2-(4-morpholinyl)ethoxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



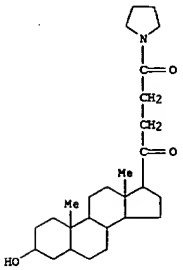
RN 38601-41-1 CAPLUS
CN Pregnane-11,20-dione, 3-hydroxy-21-[2-(4-methyl-1-piperazinyl)ethoxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1970:404089 CAPLUS
DOCUMENT NUMBER: 73:4089
TITLE: Steroids and related natural products. LI. Bufadienolides. 4. Reaction of 20-oxo steroids with methoxymethylenetriphenylphosphorane
AUTHOR(S): Pettit, George R.; Green, Brian; Dunn, George L.; Sunder-Plassmann, Paul
CORPORATE SOURCE: Dep. of Chem., Univ. of Maine, Orono, ME, USA
SOURCE: Journal of Organic Chemistry (1970), 35(5), 1385-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of 3-hydroxy-20-oxo-5-pregnenes with the ylid prepd. from methoxy-methyltriphenylphosphonium chloride was studied in detail. 3.beta.-Acetoxy-20-methoxymethylene-5-pregnene (I) was also obtained along with a comparable amt. of 3.beta.-acetoxy-26,27-dinor-5,20(22)-cholestadiene, employing the mixt. of phosphoranes from methoxymethyltri-n-butylphosphonium chloride. Acid-catalyzed hydrolysis of vinyl ether I afforded the 20-aldehyde. Attempts to condense (methoxymethylene) triphenylphosphorane with Me 3.beta.-acetoxy-20-oxo-21-nor-5, trans-22-choladienate, its cis isomer, or Me3.beta.-acetoxy-20-oxo-21-nor-5.alpha.-cholanate led to extensive side reactions attributable to the Me ester group. Use of the 3.beta.-tetrahydropyranyloxy-20-oxo-21-nor-5.alpha.-cholanic acid or tert-Bu 3.beta.-acetoxy-20-oxo-21-nor-5.alpha. cholanate or the pyrrolidine amide eliminated side reactions but satisfactory involvement of the 20-ketone was not realized.
IT **23439-96-5P 23439-97-6P 23439-98-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 23439-96-5 CAPLUS
CN Pyrrolidine, 1-(3.beta.-hydroxy-20-oxo-21-nor-5.alpha.-cholan-24-oyl)-, acetate (ester) (8CI) (CA INDEX NAME)

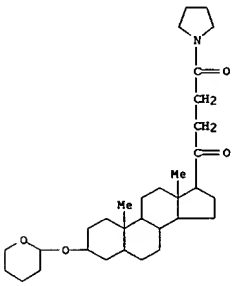


RN 23439-97-6 CAPLUS

L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Pyrrolidine, 1-(3.beta.-hydroxy-20-oxo-21-nor-5.alpha.-cholan-24-oyl)- (8CI) (CA INDEX NAME)



RN 23439-98-7 CAPLUS
CN Pyrrolidine, 1-[20-oxo-3.beta.-[(tetrahydro-2H-pyran-2-yl)oxy]-21-nor-5.alpha.-cholan-24-oyl]- (8CI) (CA INDEX NAME)



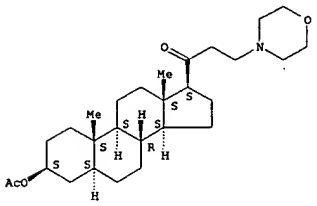
L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1962:2568 CAPLUS
DOCUMENT NUMBER: 56:2568
ORIGINAL REFERENCE NO.: 56:530c-f
TITLE: Mannich bases of steroids and their salts
INVENTOR(S): Thesing, Jan; Bork, Karl Heinz
PATENT ASSIGNEE(S): E. Merck A.-G.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 1107662 | | | DE | 19590704 |

AB 17.beta.-Acetylsteroids were treated simultaneously or in turn with CH2O and a secondary amine under the conditions of the Mannich reaction and the Mannich bases optionally treated with an acid to give the title compds. Thus, a mixt. of 7.17 5-pregnen- 3.beta.-ol-20-one acetate, 1.2 paraformaldehyde, and 2.66 g. piperdinium chloride in 100 cc. tert-amyl alc. was refluxed 4 hrs. and the soln. cooled and dild. with Et2O to give 21-piperidinomethyl-5-pregnen-3.beta.-ol-20-one. 3-acetate-HCl (I), m. 208-10.degree. (Me2CO), [.alpha.] 2Ds O .degree.; free base (II), m. 140-2.degree. (MeOH), [.alpha.]D 10.1.degree.. I on sapon. with concd. HCl gave 21-piperidinomethyl-5-pregnen-3.beta.-ol-20-one-HCl, m. 219-22.degree. (EtOH); free base (II), m. 168-70.degree.,[.alpha.]D 13.1.degree.. Similarly were prepd. the following Mannich bases or their salts (product, m. p., and [.alpha.]D given): II maleate, 154-6.degree. (Me2CO), 4.degree.; II camphorsulfonate, 193-4.degree., 15.5.degree.; II tartrate, 141.degree., III succinate, 111-20.degree., 16.0.degree. III succinate, 110-1.degree.; 21-piperidinomethyl-5,16-pregnadien-3.beta.-ol-20-one, 24.1.degree.; (EtOH), -42.6.degree.; 21-dimethylaminomethyl-5-pregnen-3.beta.-ol-20-one 3-acetate-HCl, 25.7.degree.); 21-pyrrolidinomethyl-5-pregnen-3.beta.-ol-20-one 3-acetate-HCl, 198-9.degree. [free base, 138-40.degree. (aq. EtOH); succinate 102-4.degree. (Me2CO), 9.3.degree.]; 21-morpholinomethlylallopregnan-3.beta.-ol-20-one 3-acetate-HCl, 197-9.degree. (iso-PrOH), 48.0.degree. [free base, 92-5.degree. (hexane), 56.0.degree.]; 16-methyl-21-piperidinomethyl-15-16 pregnadien-3.beta.-ol-20-one 3-acetate HCl, 213-16.degree. - [free base, 95-7.degree. (MeOH), -0.6.degree.].
IT **103572-42-5**, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-morpholino-, acetate, hydrochloride **103572-43-6**, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-morpholino-, acetate **106481-73-6**, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-piperidino-, acetate, hydrochloride **106481-74-7**, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-piperidino-, acetate
(prepn. of)
RN 103572-42-5 CAPLUS
CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-morpholino-, acetate, hydrochloride (7CI) (CA INDEX NAME)

Absolute stereochemistry.

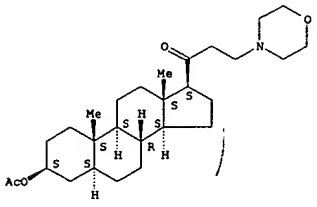
L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

RN 103572-43-6 CAPLUS
CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-morpholino-, acetate (7CI) (CA INDEX NAME)

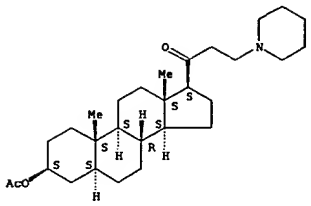
Absolute stereochemistry.



RN 106481-73-6 CAPLUS
CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-piperidino-, acetate, hydrochloride (7CI) (CA INDEX NAME)

Absolute stereochemistry.

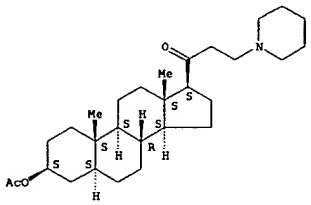
L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

RN 106481-74-7 CAPLUS
CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androstan-17.beta.-yl)-3-piperidino-, acetate (7CI) (CA INDEX NAME)

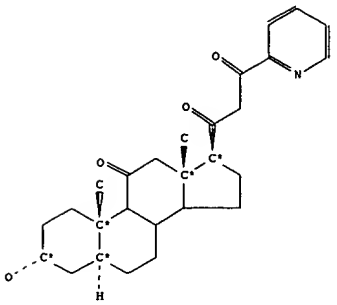
Absolute stereochemistry.



=> d all 1-13

L12 ANSWER 1 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1609851 |
| Beilstein Pref. RN (BPR): | 51227-92-0 |
| CAS Reg. No. (RN): | 51227-92-0 |
| Chemical Name (CN): | 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione |
| Autonom Name (AUN): | 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione |
| Molec. Formula (MF): | C27 H35 N O4 |
| Molecular Weight (MW): | 437.58 |
| Lawson Number (LN): | 26223 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1549260 |
| Tautomer ID (TAUTID): | 1623273 |
| Beilstein Citation (BSO): | 5-21 |
| Entry Date (DED): | 1988/11/30 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |

L12 ANSWER 1 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |
| UVS | UV and Visible Spectrum | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 179 - 180 | 1 |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 21.4 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

UV and Visible Spectrum:

| Description (.KW) | Ref. |
|---|---|
| UV/VIS | 1 |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:
RX

| | |
|---|---|
| Reaction ID (.ID): | 6850433 |
| Product BRN (.PBRN): | 1609851 |
| Product (.PRO): | 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione |
| No. of React. Details (.NVAR): | 1 |

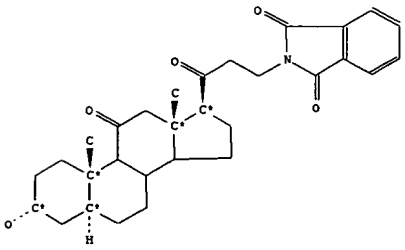
Reaction Details:
RX

| | |
|---|---|
| Reaction RID (.RID): | 6850433.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1519724 |
| Beilstein Pref. RN (BPR): | 51228-32-1 |
| CAS Reg. No. (RN): | 51228-32-1 |
| Chemical Name (CN): | 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione |
| Autonom Name (AUN): | 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione |
| Molec. Formula (MF): | C30 H37 N O5 |
| Molecular Weight (MW): | 491.63 |
| Lawson Number (LN): | 25776, 15890 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1481883 |
| Tautomer ID (TAUTID): | 1539358 |
| Beilstein Citation (BSO): | 5-21 |
| Entry Date (DED): | 1988/11/30 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 187 - 189 | 1 |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 58.8 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:
RX

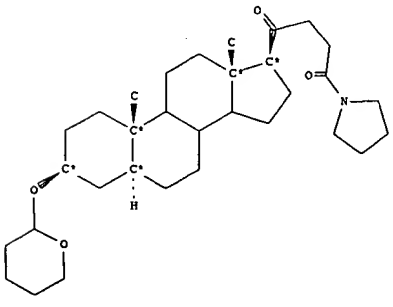
| | |
|---|---|
| Reaction ID (.ID): | 6647974 |
| Product BRN (.PBRN): | 1519724 |
| Product (.PRO): | 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:
RX

| | |
|---|---|
| Reaction RID (.RID): | 6647974.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |
| Reference(s): | |
| 1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089) | |

L12 ANSWER 3 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1412117 |
| Beilstein Pref. RN (BPR): | 23439-98-7 |
| CAS Reg. No. (RN): | 23439-98-7 |
| Chemical Name (CN): | 1-<10,13-dimethyl-3-(tetrahydro-pyran-2-yloxy)-hexadecahydro-cyclopenta<a>phenanthren-17-yl>-4-pyrrolidin-1-yl-butane-1,4-dione |
| Autonom Name (AUN): | 1-<10,13-dimethyl-3-(tetrahydro-pyran-2-yloxy)-hexadecahydro-cyclopenta<a>phenanthren-17-yl>-4-pyrrolidin-1-yl-butane-1,4-dione |
| Molec. Formula (MF): | C32 H51 N O4 |
| Molecular Weight (MW): | 513.76 |
| Lawson Number (LN): | 24077, 17122, 13467 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1392251 |
| Tautomer ID (TAUTID): | 1440908 |
| Beilstein Citation (BSO): | 5-20 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

L12 ANSWER 3 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 117 - 119 | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 65 | [alpha] | 589 | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

| Descript ion (.KW) | Ref. |
|---|---|
| IR | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 3 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Reaction:
RX

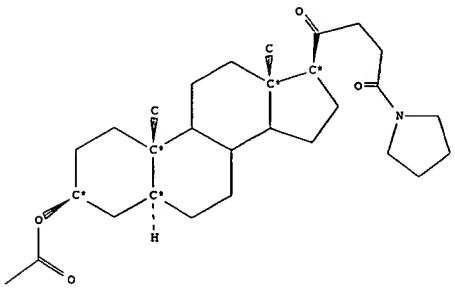
| | |
|---|---|
| Reaction ID (.ID): | 6559028 |
| Product BRN (.PBRN): | 1412117 |
| Product (.PRO): | 1-<10,13-dimethyl-3-(tetrahydro-pyran-2-yloxy)-hexadecahydro-cyclopenta<a>phenanthren-17-yl>-4-pyrrolidin-1-yl-butane-1,4-dione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:
RX

| | |
|---|---|
| Reaction RID (.RID): | 6559028.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |
| Reference(s): | |
| 1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398 | |

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1410392 |
| Beilstein Pref. RN (BPR): | 23439-96-5 |
| CAS Reg. No. (RN): | 23439-96-5 |
| Chemical Name (CN): | acetic acid 10,13-dimethyl-17-(4-oxo-4-pyrrolidin-1-yl-butyryl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester |
| Autonom Name (AUN): | acetic acid 10,13-dimethyl-17-(4-oxo-4-pyrrolidin-1-yl-butyryl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester |
| Molec. Formula (MF): | C29 H45 N O4 |
| Molecular Weight (MW): | 471.68 |
| Lawson Number (LN): | 24077, 13467, 1155 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1390379 |
| Tautomer ID (TAUTID): | 1442152 |
| Beilstein Citation (BSO): | S-20 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 124 - 125 | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

| Description (.KW) | Ref. |
|---|---|
| IR | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Reaction:
RX

| | |
|---|---|
| Reaction ID (.ID): | 6557733 |
| Product BRN (.PBRN): | 1410392 |
| Product (.PRO): | acetic acid 10,13-dimethyl-17-(4-oxo-4-pyrrolidin-1-yl-butyryl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:
RX

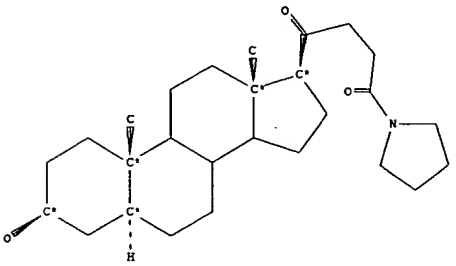
| | |
|---|---|
| Reaction RID (.RID): | 6557733.1 |

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | |
|---|---|
| Reaction Classification (.CL): | Preparation (half reaction) |
| Reference(s): | |
| 1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398 | |

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1406458 |
| Beilstein Pref. RN (BPR): | 23439-97-6 |
| CAS Reg. No. (RN): | 23439-97-6 |
| Chemical Name (CN): | 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione |
| Autonom Name (AUN): | 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione |
| Molec. Formula (MF): | C27 H43 N O3 |
| Molecular Weight (MW): | 429.64 |
| Lawson Number (LN): | 24077, 13467 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1388949 |
| Tautomer ID (TAUTID): | 1438336 |
| Beilstein Citation (BSO): | 5-20 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 222 - 224 | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 67 | [alpha] | 589 | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

| Descript ion (.KW) | Ref. |
|---|---|
| IR | 1 |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

Reaction:
RX

| | |
|---|---|
| Reaction ID (.ID): | 6554710 |
| Product BRN (.PBRN): | 1406458 |
| Product (.PRO): | 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione |
| No. of React. Details (.NVAR): | 1 |

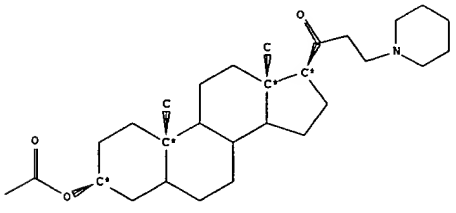
Reaction Details:
RX

| | |
|---|---|
| Reaction RID (.RID): | 6554710.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |

Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 6 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1356921 |
| Beilstein Pref. RN (BPR): | 106481-74-7 |
| CAS Reg. No. (RN): | 106481-74-7 |
| Chemical Name (CN): | 3.beta.-Acetoxy-21-piperidinomethyl-allopregnan-20-on |
| Autonom Name (AUN): | acetic acid 10,13-dimethyl-17-(3-piperidin-1-yl-propionyl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester |
| Molec. Formula (MF): | C29 H47 N O3 |
| Molecular Weight (MW): | 457.70 |
| Lawson Number (LN): | 24081, 15809, 1155 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1303936 |
| Tautomer ID (TAUTID): | 1343478 |
| Beilstein Citation (BSO): | 5-20 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1991/03/25 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| CDER | Chemical Derivative | 2 |
| FINFO | Further Information | 1 |

L12 ANSWER 6 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| MP | Melting Point | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Chemical Derivative:
CDER
Note(s) (.COM): Hydrochlorid: F: 180-182grad (Wasser)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>
CDER
Note(s) (.COM): Hydrogentartrat: F: 109-111grad (EtOH); <.alpha.>(D) +44.0grad (Dioxan)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 96 - 97 | 1 |

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

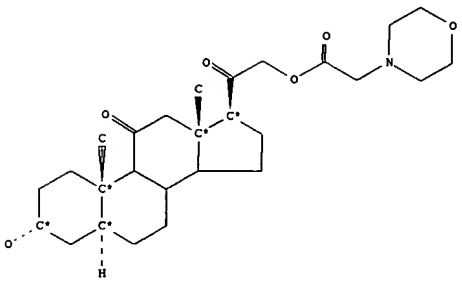
Further Information:
FINFO
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Reaction:
RX
Reaction ID (.ID): 6514830
Product BRN (.PBRN): 1356921
Product (.PRO): 3.beta.-Acetoxy-21-piperidinomethyl-allopregnan-20-on
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 6514830.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1189841
Beilstein Pref. RN (BPR): 38392-79-9
CAS Reg. No. (RN): 38392-79-9
Chemical Name (CN): 3-hydroxy-21-(morpholin-4-yl-acetoxy)-pregnane-11,20-dione
Autonom Name (AUN): morpholin-4-yl-acetic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester
Molec. Formula (MF): C27 H41 N O6
Molecular Weight (MW): 475.62
Lawson Number (LN): 30824, 9769, 3379
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 1133480
Tautomer ID (TAUTID): 1155411
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1992/04/08



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 131 - 133 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 87.5 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

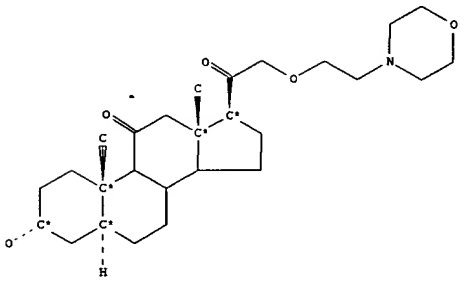
Reaction:
RX
Reaction ID (.ID): 6382297
Product BRN (.PBRN): 1189841
Product (.PRO): 3-hydroxy-21-(morpholin-4-yl-acetoxy)-pregnane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 6382297.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1182924 |
| Beilstein Pref. RN (BPR): | 38601-40-0 |
| CAS Reg. No. (RN): | 38601-40-0 |
| Chemical Name (CN): | 3-hydroxy-21-(2-morpholin-4-yl-ethoxy)-pregnane-11,20-dione |
| Autonom Name (AUN): | 3-hydroxy-10,13-dimethyl-17-<(2-morpholin-4-yl-ethoxy)-acetyl>-hexadecahydro-cyclopenta<a>phenanthren-11-one |
| Molec. Formula (MF): | C27 H43 N O5 |
| Molecular Weight (MW): | 461.64 |
| Lawson Number (LN): | 30824, 9769, 3122 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1131927 |
| Tautomer ID (TAUTID): | 1151603 |
| Beilstein Citation (BSO): | 5-27 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1992/04/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |

L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 112 - 113 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 72 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

Reaction:
RX

| | |
|---|---|
| Reaction ID (.ID): | 6377982 |
| Product BRN (.PBRN): | 1182924 |
| Product (.PRO): | 3-hydroxy-21-(2-morpholin-4-yl-ethoxy)-pregnane-11,20-dione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

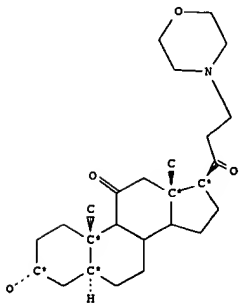
L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)
RX

| | |
|---|---|
| Reaction RID (.RID): | 6377982.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

L12 ANSWER 9 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 1176237 |
| Beilstein Pref. RN (BPR): | 51228-01-4 |
| CAS Reg. No. (RN): | 51228-01-4 |
| Chemical Name (CN): | 3-hydroxy-23-morpholin-4-yl-21,24-dinor-cholane-11,20-dione |
| Autonom Name (AUN): | 3-hydroxy-10,13-dimethyl-17-(3-morpholin-4-yl-propionyl)-hexadecahydro-cyclopenta<a>phenanthren-11-one |
| Molec. Formula (MF): | C26 H41 N O4 |
| Molecular Weight (MW): | 431.61 |
| Lawson Number (LN): | 30824, 15890 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 1131471 |
| Tautomer ID (TAUTID): | 1150123 |
| Beilstein Citation (BSO): | 5-27 |
| Entry Date (DED): | 1988/11/29 |
| Update Date (DUPD): | 1992/04/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |

L12 ANSWER 9 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 73 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:
RX
Reaction ID (.ID): 6373933
Product BRN (.PBRN): 1176237
Product (.PRO): 3-hydroxy-23-morpholin-4-yl-21,24-dinor-cholane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 6373933.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 10 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

| | | |
|---|---|---|
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 84.5 | [alpha] | 589 | 1 |

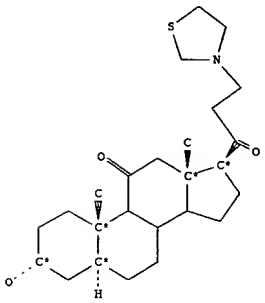
Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:
RX
Reaction ID (.ID): 6372577
Product BRN (.PBRN): 1174057
Product (.PRO): 3-hydroxy-23-thiazolidin-3-yl-21,24-dinor-cholane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 6372577.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 10 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1174057
Beilstein Pref. RN (BPR): 51228-28-5
CAS Reg. No. (RN): 51228-28-5
Chemical Name (CN): 3-hydroxy-23-thiazolidin-3-yl-21,24-dinor-cholane-11,20-dione
Autonom Name (AUN): 3-hydroxy-10,13-dimethyl-17-(3-thiazolidin-3-yl-propionyl)-hexadecahydro-cyclopenta<a>phenanthren-11-one
Molec. Formula (MF): C25 H39 N O3 S
Molecular Weight (MW): 433.65
Lawson Number (LN): 30831, 15890
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 1128524
Tautomer ID (TAUTID): 1149485
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1992/04/08

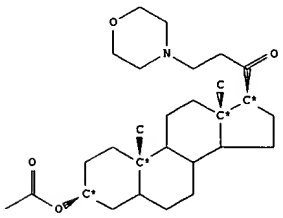


Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1047630
Beilstein Pref. RN (BPR): 103572-43-6
CAS Reg. No. (RN): 103572-43-6
Chemical Name (CN): 3-acetoxy-23-morpholin-4-yl-21,24-dinor-cholan-20-one
Autonom Name (AUN): acetic acid 10,13-dimethyl-17-(3-morpholin-4-yl-propionyl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester
Molec. Formula (MF): C28 H45 N O4
Molecular Weight (MW): 459.67
Lawson Number (LN): 30824, 15809, 1155
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 1026819
Tautomer ID (TAUTID): 1046176
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1992/04/07



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| UPD | Update Date | 1 |
| CDER | Chemical Derivative | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Chemical Derivative:
CDER
Note(s) (.COM): Hydrochlorid: F: 197-199grad (Propan-2-ol); <.alpha.>(D): +48.0grad (Dioxan)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Melting Point:

| Value (MP) (Cel) | Solvent (.SOL) | Ref. |
|---|---|---|
| 92 - 95 | hexane | 1 |

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Solvent (.SOL) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|---|
| 56 | [alpha] | dioxane | 589 | 1 |

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

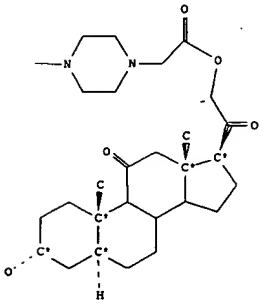
Reaction:
RX
Reaction ID (.ID): 6301110
Product BRN (.PBRN): 1047630
Product (.PRO): 3-acetoxy-23-morpholin-4-yl-21,24-dinor-cholan-20-one
No. of React. Details (.NVAR): 1

Reaction Details:

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)
RX
Reaction RID (.RID): 6301110.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 867726
Beilstein Pref. RN (BPR): 38392-80-2
CAS Reg. No. (RN): 38392-80-2
Chemical Name (CN): 3-hydroxy-21-<(4-methyl-piperazin-1-yl)-acetoxy>-pregnane-11,20-dione, (4-methyl-piperazin-1-yl)-acetic acid 3-hydroxy-11,20-dioxo-pregnan-21-yl ester
Autonom Name (AUN): (4-methyl-piperazin-1-yl)-acetic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester
Molec. Formula (MF): C28 H44 N2 O5
Molecular Weight (MW): 488.67
Lawson Number (LN): 28000, 9769, 3379, 2817
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 844542
Tautomer ID (TAUTID): 864337
Beilstein Citation (BSO): 5-23
Entry Date (DED): 1988/11/28
Update Date (DUPD): 1989/12/04



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 2 |
| AUN | Autonomname | 1 |

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 4 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 158 - 163 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 83 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

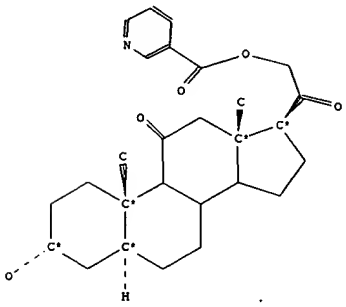
Reaction:
RX
Reaction ID (.ID): 6153907
Product BRN (.PBRN): 867726
Product (.PRO): 3-hydroxy-21-<(4-methyl-piperazin-1-yl)-acetoxy>-pregnane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 6153907.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

| | |
|---|---|
| Beilstein Records (BRN): | 463947 |
| Beilstein Pref. RN (BPR): | 38392-72-2 |
| CAS Reg. No. (RN): | 38392-72-2 |
| Chemical Name (CN): | nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester |
| Autonom Name (AUN): | nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester |
| Molec. Formula (MF): | C27 H35 N O5 |
| Molecular Weight (MW): | 453.58 |
| Lawson Number (LN): | 26332, 9769 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 454285 |
| Tautomer ID (TAUTID): | 472546 |
| Beilstein Citation (BSO): | 5-22 |
| Entry Date (DED): | 1988/11/28 |
| Update Date (DUPD): | 1988/12/08 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

| | | |
|---|---|---|
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| MP | Melting Point | 1 |
| ORP | Optical Rotatory Power | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

Melting Point:

| Value (MP) (Cel) | Ref. |
|---|---|
| 208 - 211 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

| Value (ORP) (deg) | Type (.TYP) | Wavelen. (.W) (nm) | Ref. |
|---|---|---|---|
| 110.5 | [alpha] | 589 | 1 |

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Reaction:
RX

| | |
|---|---|
| Reaction ID (.ID): | 5666708 |
| Product BRN (.PBRN): | 463947 |
| Product (.PRO): | nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)
RX

| | |
|---|---|
| Reaction RID (.RID): | 5666708.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

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=> d his

     (FILE 'HOME' ENTERED AT 11:49:17 ON 23 SEP 2003)

     FILE 'REGISTRY'. ENTERED AT 11:49:25 ON 23 SEP 2003
L1                STRUCTURE UPLOADED
L2             0 S L1
L3            77 S L1 FULL
L4                STRUCTURE UPLOADED
L5            10 S L4 FULL SUB=L3
L6            10 S L4 FULL
L7                STRUCTURE UPLOADED
L8            19 S L7 FULL
L9            29 S L6 OR L8

     FILE 'CAPLUS' ENTERED AT 11:59:19 ON 23 SEP 2003
L10            9 S L8

     FILE 'BEILSTEIN' ENTERED AT 12:03:14 ON 23 SEP 2003
L11            0 S L4 FULL
L12           13 S L7 FULL
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L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:790531 CAPLUS
DOCUMENT NUMBER: 133:350392
TITLE: Preparation of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity
INVENTOR(S): Hogenkamp, Derk L.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000066614 | A1 | 20001109 | WO 2000-US11680 | 20000428 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| BR 2000010060 | A | 20020115 | BR 2000-10060 | 20000428 |
| EP 1177206 | A1 | 20020206 | EP 2000-930250 | 20000428 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002543218 | T2 | 20021217 | JP 2000-615643 | 20000428 |
| NO 2001005262 | A | 20011219 | NO 2001-5262 | 20011026 |

PRIORITY APPLN. INFO.: US 1999-131578P P 19990429
WO 2000-US11680 W 20000428

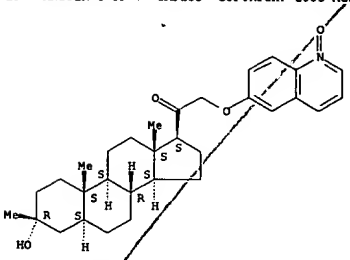
AB 3.alpha.-Hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids I (R1 = H, Me; R2 = 5.alpha.- or 5.beta.-H; R3 = optionally substituted N-attached heteroaryl group or -XR4 where R4 = optionally substituted carbon-attached heteroaryl group; X = O, S, N) or a pharmaceutically acceptable salt, prodrug or solvate thereof were prepd. Thus II was prepd. from 3.alpha.-hydroxy-3.beta.-methoxymethyl-5.alpha.-pregnan-20-one and imidazole which was then converted to the hydrochloride salt. Steroids I are useful as anticonvulsants, sedative/hypnotics and anesthetics {no data}.

IT 304910-83-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity)

RN 304910-83-6 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-(6-quinolinyloxy)-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

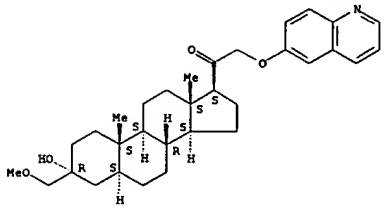
Absolute stereochemistry.

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

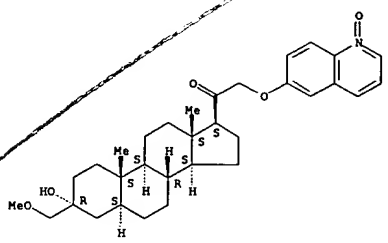
L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 256955-85-8P 304910-84-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity)

RN 256955-85-8 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 304910-84-7 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:778442 CAPLUS
DOCUMENT NUMBER: 132:132237
TITLE: Response-rate suppression in operant paradigm as predictor of soporific potency in rats and identification of three novel sedative-hypnotic neuroactive steroids
AUTHOR(S): Vanover, Kimberly E.; Edgar, Dale M.; Seidel, Wesley F.; Hogenkamp, Derk J.; Fick, David B.; Lan, Nancy C.; Gee, Kelvin W.; Carter, Richard B.
CORPORATE SOURCE: CoCensys, Inc., Irvine, CA, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1999), 291(3), 1317-1323
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

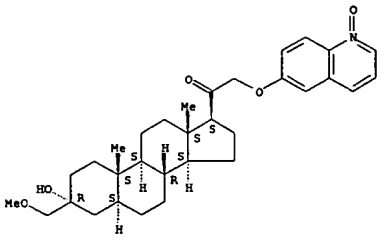
AB Novel neuroactive steroids were evaluated for their effects on operant responding, rotorod motor performance, and EEG recording in rats. Co 134444, Co 177843, and Co 127501 were compared with the prototypical .gamma.-aminobutyric acidA-pos. allosteric modulators triazolam, zolpidem, pentobarbital, pregnanolone, and CCD 3693. Each of the compds. produced a dose-related decrease in response rates under a variable-interval 2-min schedule of pos. reinforcement in an operant paradigm. In addn., all compds. produced a dose-related increase in ataxia and significant increases in nonrapid eye movement sleep in this expt. or have been previously reported to do so. Co 134444, Co 177843, and Co 127501 increased nonrapid eye movement sleep at doses that had no effect on rapid eye movement sleep. All of the compds. were more potent at decreasing operant responding than they were at increasing ataxia. Furthermore, the potency of compds. to produce response-rate suppression in an operant paradigm appeared to be a better predictor of soporific potency than did potency in the rotorod assay. The screening for sedative-hypnotic activity resulted in the identification of the novel orally active neuroactive steroids Co 134444, Co 177843, and Co 127501.

IT 256955-85-8, Co 177843
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(response-rate suppression in operant paradigm as predictor of soporific potency: novel sedative-hypnotic neuroactive steroids identification)

RN 256955-85-8 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

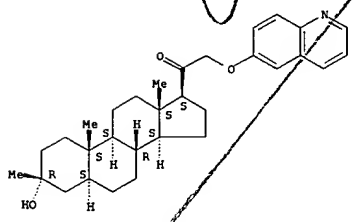
Absolute stereochemistry.

L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:450892 CAPLUS
DOCUMENT NUMBER: 131:102428
TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: U.S., 28 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5925630 | A | 19990720 | US 1996-659192 | 19960606 |
| CA 2223996 | AA | 19961219 | CA 1996-2223996 | 19960606 |
| CN 1190404 | A | 19980812 | CN 1996-195360 | 19960606 |
| EP 1288220 | A2 | 20030305 | EP 2002-25321 | 19960606 |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL

PRIORITY APPLN. INFO.: US 1995-467404 A2 19950606
EP 1996-919372 A3 19961219
OTHER SOURCE(S): MARPAT 131:102428

AB Neuroactive steroids of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halo, alkoxy, alkyl, alkenyl, alkynyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, aryl, etc.; R2 = H, alkoxy, keto, Me2N; R3 = alkoxy, alkenyloxy, alkynyloxy; R4 = H, Me; R5 = H, absent; R6 = H, alkanoyl, etc.; R7 = H, halo, OH, alkoxy, etc.; R8 = H, halo; R9 = H, halo, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halo, alkyl, OH, alkoxy, CN, etc.] are prepd. These derivs. are capable of acting at a recently identified site on the GABA receptor complex (GRC), thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.beta.-methoxy-5.beta.-androstan-3-one to give II. II protected 87.5% of mice injected with metrazol from convulsions.

IT **186264-63-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neuroactive steroids of androstane and pregnane series)

RN 186264-63-1 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:112239 CAPLUS
DOCUMENT NUMBER: 128:188632
TITLE: Use of GABA agonists and NMDA receptor antagonists for the treatment of migraine headache
INVENTOR(S): Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA; Lan, Nancy C.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9805337 | A1 | 19980212 | WO 1997-US13430 | 19970731 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9739672 | A1 | 19980225 | AU 1997-39672 | 19970731 |

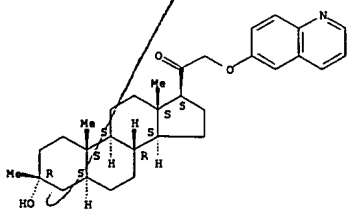
PRIORITY APPLN. INFO.: US 1996-22937P P 19960801
WO 1997-US13430 W 19970731

AB Methods are disclosed for treating or preventing migraine headache by administering to an animal a GABA receptor agonist (e.g. a neuroactive steroid) and/or an NMDA receptor antagonist (e.g. a dihydroquinoxaline deriv.). Also disclosed are pharmaceutical compns. and kits for the treatment or prevention of migraine headache.

IT **186264-63-1 203719-40-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(GABA agonists and NMDA receptor antagonists for migraine headache treatment)

RN 186264-63-1 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

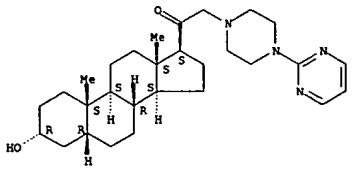
Absolute stereochemistry.



L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 203719-40-8 CAPLUS
CN Pregnan-20-one, 3-hydroxy-21-[4-(2-pyrimidinyl)-1-piperazinyl]-, (3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

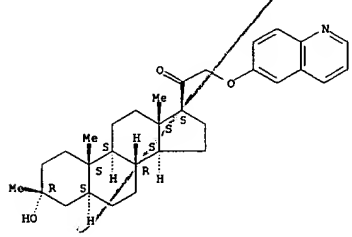
L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

5.beta.-androstan-3-one to give II. II (10 mg/kg IP) protected 87.5% of mice injected with metrazol from convulsions.

IT **186264-63-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neuroactive androstanes and pregnanes)

RN 186264-63-1 CAPLUS
CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:113460 CAPLUS
DOCUMENT NUMBER: 126:131695
TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9640043 | A2 | 19961219 | WO 1996-US10115 | 19960606 |
| WO 9640043 | A3 | 19970327 | | |
| W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN | | | | |
| CA 2223996 | AA | 19961219 | CA 1996-2223996 | 19960606 |
| AU 9661725 | A1 | 19961230 | AU 1996-61725 | 19960606 |
| AU 725214 | B2 | 20001005 | | |
| EP 837874 | A2 | 19980429 | EP 1996-919372 | 19960606 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI | | | | |
| CN 1190404 | A | 19980812 | CN 1996-195360 | 19960606 |
| BR 9608592 | A | 19990629 | BR 1996-8592 | 19960606 |
| JP 11507643 | T2 | 19990706 | JP 1997-502210 | 19960606 |
| RU 2194712 | C2 | 20021220 | RU 1998-100755 | 19960606 |
| EP 1288220 | A2 | 20030305 | EP 2002-25321 | 19960606 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL | | | | |
| NO 9705608 | A | 19980206 | NO 1997-5608 | 19971204 |
| FI 9704448 | A | 19971205 | FI 1997-4448 | 19971205 |

PRIORITY APPLN. INFO.: US 1995-467404 A 19950606
WO 1996-US10115 W 19960606
EP 1996-919372 A3 19961219

OTHER SOURCE(S): MARPAT 126:131695

AB Compds. of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halogen, alkoxy, alkyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R2 = H, OH, alkoxy, alkanoyloxy, carbalkoxy, keto, amino; R3 = H, alkoxy, alkenyloxy, etc.; R4 = H, alkyl; R5 = H, absent; R6 = H, alkanoyl, aminocarbonyl, alkoxycarbonyl; R7 = H, halogen, OH, alkoxy, alkanoyloxy, carbalkoxy; R8 = H, halogen; R9 = H, halogen, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halogen, OH, alkyl, etc.] are prepd. as neuroactive prodrugs, due to their ability to modulate the GABAA receptor-chloride ionophore complex. These derivs. are capable of acting at a recently identified site on the GRC, thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.beta.-methoxy-

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1988:631361 CAPLUS
DOCUMENT NUMBER: 109:231361
TITLE: Amino steroids useful for treating a variety of conditions, and a process for their preparation
INVENTOR(S): McCall, John M.; Ayer, Donald E.; Jacobsen, E. Jon; Van Doorick, Frederick J.; Palmer, John R.; Karnes, Harold A.
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: Eur. Pat. Appl., 90 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 263213 | A1 | 19880413 | EP 1986-307808 | 19861009 |
| EP 263213 | B1 | 19950906 | | |
| R: AT, ES, GR | | | | |
| ES 2078890 | T3 | 19960101 | ES 1986-307808 | 19861009 |

PRIORITY APPLN. INFO.: EP 1986-307808 19861009

OTHER SOURCE(S): CASREACT 109:231361; MARPAT 109:231361

AB Various amino-substituted steroids were prepd. for use in the treatment of a wide variety of conditions. Aminolysis of 21-iodo-16.alpha.-methylpregna-1,4,9(11)-triene-3,20-dione by 1-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)piperazine in MeCN contg. K2CO3 at 60.degree., followed by chromatog. and salification with MeSO3H, gave the amino steroid dimethanesulfonate I. In the in vivo mouse head injury test of Hall, 3 mg I/kg increases 1-h post-injury grip test scores by 134.5%.

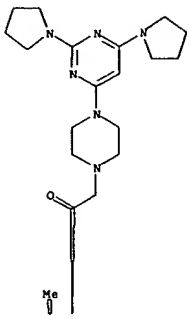
IT **111641-00-0P 111641-01-1P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)

RN 111641-00-0 CAPLUS
CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.beta.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

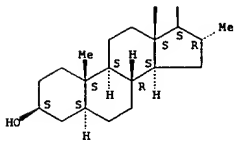
Absolute stereochemistry.

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

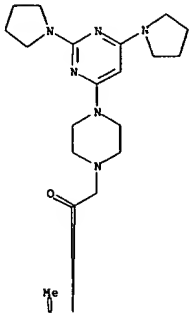


RN 111641-01-1 CAPLUS
CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.alpha.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

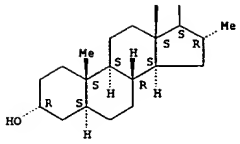
Absolute stereochemistry.

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1988:6287 CAPLUS
DOCUMENT NUMBER: 108:6287
TITLE: Amino-substituted steroids having a variety of pharmacological activities, and processes for their preparation
INVENTOR(S): McCall, John M.; Jacobsen, E. Jon; Van Doornik, Frederick J.; Palmer, John R.; Karnes, Harold A.
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 8701706 | A2 | 19870326 | WO 1986-US1797 | 19860828 |
| WO 8701706 | A3 | 19870716 | | |
| W: AU, DK, FI, JP, KR, NO, SU, US, US, US, US | | | | |
| RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| IL 79702 | A1 | 19920216 | IL 1986-79702 | 19860812 |
| IL 98007 | A1 | 19920216 | IL 1986-98007 | 19860812 |
| ZA 8606097 | A | 19880330 | ZA 1986-6097 | 19860813 |
| CA 1308707 | A1 | 19921013 | CA 1986-516177 | 19860818 |
| AU 8663356 | A1 | 19870407 | AU 1986-63356 | 19860828 |
| AU 593284 | B2 | 19900208 | | |
| EP 238545 | A1 | 19870930 | EP 1986-905605 | 19860828 |
| EP 238545 | B1 | 19951115 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| JP 63500868 | T2 | 19880331 | JP 1986-504810 | 19860828 |
| JP 05035158 | B4 | 19930525 | | |
| AT 130307 | E | 19951215 | AT 1986-905605 | 19860828 |
| CN 86106226 | A | 19870318 | CN 1986-106226 | 19860912 |
| CN 1030319 | B | 19951122 | | |
| DK 8702375 | A | 19870511 | DK 1987-2375 | 19870511 |
| NO 8701930 | A | 19870511 | NO 1987-1930 | 19870511 |
| NO 176762 | B | 19950213 | | |
| NO 176762 | C | 19950531 | | |
| FI 8702107 | A | 19870512 | FI 1987-2107 | 19870512 |
| FI 94417 | B | 19950531 | | |
| FI 94417 | C | 19950911 | | |
| US 5099019 | A | 19920324 | US 1988-229675 | 19880808 |
| AU 8940806 | A1 | 19891207 | AU 1989-40806 | 19890825 |
| AU 614661 | B2 | 19910905 | | |
| AU 8940807 | A1 | 19891207 | AU 1989-40807 | 19890825 |
| AU 614418 | B2 | 19910829 | | |
| US 5175281 | A | 19921229 | US 1991-749830 | 19910826 |
| US 5322943 | A | 19940621 | US 1991-749829 | 19910826 |
| JP 05112597 | A2 | 19930507 | JP 1992-8428 | 19920121 |
| US 35053 | E | 19951010 | US 1992-959310 | 19921009 |
| US 5268477 | A | 19931207 | US 1992-977768 | 19921119 |
| US 5380839 | A | 19950110 | US 1992-983082 | 19921201 |
| US 5380840 | A | 19950110 | US 1992-983084 | 19921201 |
| US 5380841 | A | 19950110 | US 1992-984299 | 19921201 |
| US 5382661 | A | 19950117 | US 1992-984298 | 19921201 |
| US 5506354 | A | 19960409 | US 1992-984302 | 19921201 |
| PRIORITY APPLN. INFO.: | | | US 1985-775204 | 19850912 |
| | | | US 1985-811058 | 19851219 |
| | | | US 1986-877287 | 19860623 |

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

| | | |
|---|---|---|
| | US 1986-888231 | 19860729 |
| | IL 1986-79702 | 19860812 |
| | WO 1986-US1797 | 19860828 |
| | US 1987-121822 | 19870511 |
| | US 1988-227812 | 19880803 |
| | US 1988-229675 | 19880808 |
| | US 1991-749829 | 19910826 |
| | US 1991-749830 | 19910826 |

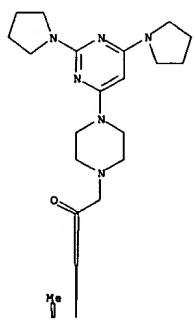
AB Numerous pregnane derivs. with amino-substituted sidechains were prepd. for use as various types of drugs. Aminolysis of 21-iodo-16.alpha.-methylpregna-1,4,9(11)-triene-3,20-dione with 4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)piperazine in MeCN contg. K2CO3 at 60.degree. gave [[bis(pyrrolidino)pyrimidinyl]piperazinyl]pregnane deriv. I, which was converted to I.2MeSO3H (II). In the interleukin-1-induced T-cell proliferation assay, II gave 62% inhibition at 10-6 M, thereby demonstrating antiarthritic activity.

IT **111641-00-0P 111641-01-1P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)

RN 111641-00-0 CAPLUS
CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.beta.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

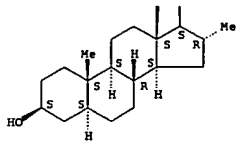
Absolute stereochemistry.

PAGE 1-A



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

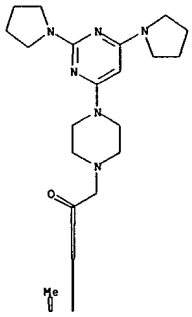
PAGE 2-A



RN 111641-01-1 CAPLUS
CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.alpha.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

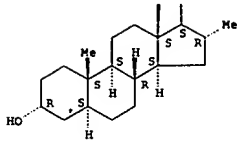
Absolute stereochemistry.

PAGE 1-A



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A



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L3             138 S L1 FULL
L4               7 S L3 AND (PYRIDY? OR PYRIMIDINY? OR PYRAZINY? OR IMIDAZOLY? OR

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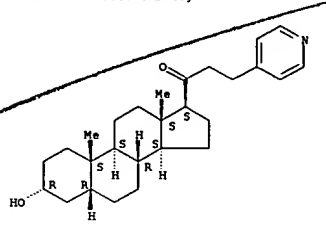
L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:113460 CAPLUS
DOCUMENT NUMBER: 126:131695
TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9640043 | A2 | 19961219 | WO 1996-US10115 | 19960606 |
| WO 9640043 | A3 | 19970327 | | |
| W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN | | | | |
| CA 2223996 | AA | 19961219 | CA 1996-2223996 | 19960606 |
| AU 9661725 | A1 | 19961230 | AU 1996-61725 | 19960606 |
| AU 725214 | B2 | 20001005 | | |
| EP 837874 | A2 | 19980429 | EP 1996-919372 | 19960606 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI | | | | |
| CN 1190404 | A | 19980812 | CN 1996-195360 | 19960606 |
| BR 9608592 | A | 19990629 | BR 1996-8592 | 19960606 |
| JP 11507643 | T2 | 19990706 | JP 1997-502210 | 19960606 |
| RU 2194712 | C2 | 20021220 | RU 1998-100755 | 19960606 |
| EP 1288220 | A2 | 20030305 | EP 2002-25321 | 19960606 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL | | | | |
| NO 9705608 | A | 19980206 | NO 1997-5608 | 19971204 |
| FI 9704448 | A | 19971205 | FI 1997-4448 | 19971205 |

PRIORITY APPLN. INFO.: US 1995-467404 A 19950606
WO 1996-US10115 W 19960606
EP 1996-919372 A3 19961219
OTHER SOURCE(S): MARPAT 126:131695
AB Compds. of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halogen, alkoxy, alkyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R2 = H, OH, alkoxy, alkanoyloxy, carbalkoxy, keto, amino; R3 = H, alkoxy, alkenyloxy, etc.; R4 = H, alkyl; R5 = H, absent; R6 = H, alkanoyl, aminocarbonyl, alkoxycarbonyl; R7 = H, halogen, OH, alkoxy, alkanoyloxy, carbalkoxy; R8 = H, halogen; R9 = H, halogen, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halogen, OH, alkyl, etc.] are prepd. as neuroactive prodrugs, due to their ability to modulate the GABAA receptor-chloride ionophore complex. These derivs. are capable of acting at a recently identified site on the GRC, thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.beta.-methoxy-

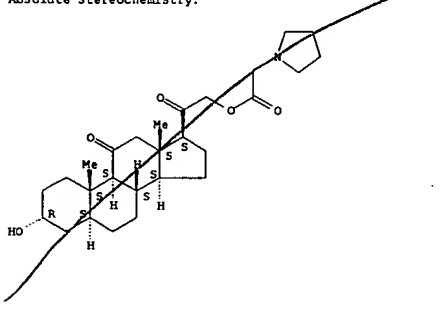
L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
5.beta.-androstan-3-one to give II. II (10 mg/kg IP) protected 87.5% of mice injected with metrazol from convulsions.
IT 186264-69-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neuroactive androstanes and pregnanes)
RN 186264-69-7 CAPLUS
CN 1-Propanone, 1-[(3.alpha.,5.beta.,17.beta.)-3-hydroxyandrostan-17-yl]-3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:558163 CAPLUS
DOCUMENT NUMBER: 83:158163
TITLE: Structure-activity relations in steroidal anesthetics
AUTHOR(S): Phillipps, G. H.
CORPORATE SOURCE: Org. Chem. Dep., Glaxo Res. Ltd., Greenford/Middlesex, UK
SOURCE: Journal of Steroid Biochemistry (1975), 6(5), 607-13
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The introduction of double bonds and substituents into Alphaxalone [23930-19-0] modify its anesthetic activity, as detd. in mice, and these modifications are discussed with particular ref. to the conformation of the A-ring. A variety of side chains may be present at the 17.beta.-position. Some water-sol. steroids which show instantaneous induction of anesthesia are described.
IT 56857-38-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anesthetic activity of)
RN 56857-38-6 CAPLUS
CN Pregnane-11,20-dione, 3-hydroxy-21-[(1-pyrrolidinylacetyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

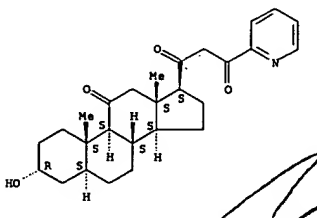


L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1974:60089 CAPLUS
DOCUMENT NUMBER: 80:60089
TITLE: 3.alpha.-Hydroxy- 5.alpha.-pregnanes
INVENTOR(S): Phillips, Gordon Hanley; Lawrence, Robin; Stephenson, Leslie; Ayres, Barry E.
PATENT ASSIGNEE(S): Glaxo Laboratories Ltd.
SOURCE: Ger. Offen., 75 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2323950 | A1 | 19731213 | DE 1973-2323950 | 19730511 |
| US 3998829 | A | 19761221 | US 1973-358381 | 19730508 |
| BE 799433 | A1 | 19731112 | BE 1973-131031 | 19730511 |
| NL 7306606 | A | 19731114 | NL 1973-6606 | 19730511 |
| FR 2184711 | A1 | 19731228 | FR 1973-17079 | 19730511 |
| JP 49048652 | A2 | 19740511 | JP 1973-52424 | 19730511 |
| ZA 7303218 | A | 19740529 | ZA 1973-3218 | 19730511 |
| AU 7355616 | A1 | 19741114 | AU 1973-55616 | 19730511 |
| GB 1436324 | A | 19760519 | GB 1972-22489 | 19730511 |
| DK 135775 | B | 19770620 | DK 1973-2604 | 19730511 |
| CA 1014947 | A1 | 19770802 | CA 1973-171026 | 19730511 |

PRIORITY APPLN. INFO.: GB 1972-22489 19720512
AB Hydroxypregnanes I, II (R = H, alkyl, acyl; R1 = H; RR1 = CH2, CH2CH2, O; R2 = H, R3 = alkoxy, alkylthio, acyl, acyloxy, acylthio, morpholino, halo, Me; R2 = R3 = Me) (45 compds.) were prepd. from I and II (R = R1 = H; R2R3 = CH2; R2 = H, R3 = CH2OH) by Claisen condensation with active methylene compds. Thus, 1 g I (R = R1 = H) was treated with AcOEt-NaH to give 0.5 g I (R1 = Ac).
IT 51227-92-0P 51228-01-4P 51228-28-5P 51228-32-1P 51228-33-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51227-92-0 CAPLUS
CN 1,3-Propanedione, 1-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51228-01-4 CAPLUS